

Time-stepping error bounds for fractional diffusion problems with non-smooth initial data

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Abstract

We apply the piecewise constant, discontinuous Galerkin method to discretize a fractional diffusion equation with respect to time. Using Laplace transform techniques, we show that the method is first order accurate at the n th time level t_n , but the error bound includes a factor t_n^{-1} if we assume no smoothness of the initial data. We also show that for smoother initial data the growth in the error bound as t_n decreases is milder, and in some cases absent altogether. Our error bounds generalize known results for the classical heat equation and are illustrated for a model problem.

Keywords: Discontinuous Galerkin method, implicit Euler method, Laplace transform, polylogarithm.

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1. Introduction

Consider an initial-value problem for an abstract, time-fractional diffusion equation [7, p. 84]

$$\partial_t u + \partial_t^{1-\nu} A u = 0 \quad \text{for } t > 0, \quad \text{with } u(0) = u_0 \text{ and } 0 < \nu < 1. \quad (1)$$

Here, we think of the solution u as a function from $[0, \infty)$ to a Hilbert space \mathcal{H} , with $\partial_t u = u'(t)$ the usual derivative with respect to t , and with

$$\partial_t^{1-\nu} u(t) = \frac{\partial}{\partial t} \int_0^t \frac{(t-s)^{\nu-1}}{\Gamma(\nu)} u(s) ds$$

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the Riemann–Liouville fractional derivative of order $1-\nu$. The linear operator A is assumed to be self-adjoint, positive-semidefinite and densely defined in \mathcal{H} , with a complete orthonormal eigensystem $\phi_1, \phi_2, \phi_3, \dots$. We further assume that the eigenvalues of A tend to infinity. Thus,

$$A\phi_m = \lambda_m\phi_m, \quad \langle \phi_m, \phi_n \rangle = \delta_{mn}, \quad 0 \leq \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots,$$

where $\langle u, v \rangle$ is the inner product in \mathcal{H} ; the corresponding norm in \mathcal{H} is denoted by $\|u\| = \sqrt{\langle u, u \rangle}$. In particular, we may take $Au = -\nabla^2 u$ and $\mathcal{H} = L_2(\Omega)$ for a bounded spatial domain Ω , with u subject to homogeneous Dirichlet or Neumann boundary conditions on $\partial\Omega$. Our problem (1) then reduces to the classical heat equation when $\nu \rightarrow 1$.

Many authors have studied techniques for the time discretization of (1), but obtaining sharp error bounds has proved challenging. In studies of explicit and implicit finite difference schemes [1, 3, 8, 14, 17, 20] the error analyses typically assume that the solution $u(t)$ is sufficiently smooth, including at $t = 0$, which amounts to imposing compatibility conditions on the initial data and source term. In our earlier work on discontinuous Galerkin (DG) time-stepping [11, 15, 16], we permitted more realistic behaviour, allowing the derivatives of $u(t)$ to be unbounded as $t \rightarrow 0$, but were seeking error bounds that are uniform in t using variable time steps. In the present work, we again consider a piecewise-constant DG scheme but with a completely different method of analysis that leads to sharp error bounds even for non-smooth initial data, at the cost of requiring a constant time step Δt . Our previous analysis [11, Theorem 5] of the scheme (5), in conjunction with relevant estimates [10] of the derivatives of u , shows, in the special case of uniform time steps, only the sub-optimal error bound

$$\|U^n - u(t_n)\| \leq C\Delta t^{r\nu} \|A^r u_0\| \quad \text{for } 0 \leq r < 1/\nu. \quad (2)$$

In our main result, we substantially improve on (2) by showing that

$$\|U^n - u(t_n)\| \leq Ct_n^{r\nu-1} \Delta t \|A^r u_0\| \quad \text{for } 0 \leq r \leq \min(2, 1/\nu). \quad (3)$$

Thus, for a general $u_0 \in \mathcal{H}$ the error is of order $t_n^{-1} \Delta t$ at $t = t_n$, so the method is first-order accurate but the error bound includes a factor t_n^{-1} that grows if t_n approaches zero, until at $t = t_1$ the bound is of order $t_1^{-1} \Delta t = 1$. However, if $1/2 \leq \nu < 1$ and u_0 is smooth enough to belong to $D(A^{1/\nu})$, the domain of $A^{1/\nu}$, then the error is of order Δt , uniformly in t_n . For $0 < \nu \leq 1/2$, no matter how smooth u_0 a factor t_n^{2r-1} is present. To the best of our knowledge, only Cuesta et al. [2] and McLean and Thomée [12, Theorem 3.1] have hitherto investigated the time discretization of (1) for the interesting case when the initial data might not be regular, the former using a finite difference-convolution quadrature scheme and the latter a method based on numerical inversion of the Laplace transform.

In the present work, we do not discuss the spatial discretization of (1). By contrast, Jin, Lazarov and Zhou [6] applied a piecewise linear finite element method using a quasi-uniform partition of Ω into elements with maximum diameter h , but with no time discretization. They worked with an equivalent

formulation of the fractional diffusion problem,

$$\partial_{t,C}^\nu u - \nabla^2 u = 0 \quad \text{for } x \in \Omega \text{ and } 0 < t \leq T, \quad (4)$$

where $\partial_{t,C}$ denotes the Caputo fractional derivative, and proved [6, Theorems 3.5 and 3.7] that, for an appropriate choice of $u_h(0)$,

$$\|u_h(t) - u(t)\| + h\|\nabla(u_h - u)\| \leq Ct^{\nu(r-1)} \times \begin{cases} h^2 \ell_h \|A^r u_0\|, & r \in \{0, 1/2\}, \\ h^2 \|A^r u_0\|, & r = 1, \end{cases}$$

where $\ell_h = \max(1, \log h^{-1})$. These estimates for the spatial error complement our bounds for the error in a time discretization.

For a fixed step size $\Delta t > 0$, we put $t_n = n\Delta t$ and define a piecewise-constant approximation $U(t) \approx u(t)$ by applying the DG method [11, 13],

$$U^n - U^{n-1} + \int_{t_{n-1}}^{t_n} \partial_t^{1-\nu} AU(t) dt = 0 \quad \text{for } n \geq 1, \text{ with } U^0 = u_0, \quad (5)$$

where $U^n = U(t_n^-) = \lim_{t \rightarrow t_n^-} U(t)$ denotes the one-sided limit from below at the n th time level. Thus, $U(t) = U^n$ for $t_{n-1} < t \leq t_n$. Since we do not consider any spatial discretization, U is a semidiscrete solution with values in \mathcal{H} . A short calculation reveals that

$$\int_{t_{n-1}}^{t_n} \partial_t^{1-\nu} AU(t) dt = \Delta t^\nu \sum_{j=1}^n \beta_{n-j} AU^j,$$

with

$$\beta_0 = \Delta t^{-\nu} \int_{t_{n-1}}^{t_n} \frac{(t_n - t)^{\nu-1}}{\Gamma(\nu)} dt = \frac{1}{\Gamma(1 + \nu)}$$

and, for $j \geq 1$,

$$\beta_j = \Delta t^{-\nu} \int_{t_{n-j-1}}^{t_{n-j}} \frac{(t_n - t)^{\nu-1} - (t_{n-1} - t)^{\nu-1}}{\Gamma(\nu)} dt = \frac{(j+1)^\nu - 2j^\nu + (j-1)^\nu}{\Gamma(1 + \nu)}.$$

Thus, by solving the recurrence relation

$$(I + \beta_0 \Delta t^\nu A)U^n = U^{n-1} - \Delta t^\nu \sum_{j=1}^{n-1} \beta_{n-j} AU^j \quad (6)$$

for $n = 1, 2, 3, \dots$ we may compute U^1, U^2, U^3, \dots .

In the classical limit as $\nu \rightarrow 1$, the fractional-order equation (1) reduces to an abstract heat equation,

$$\partial_t u + Au = 0 \quad \text{for } t > 0, \quad \text{with } u(0) = u_0, \quad (7)$$

and the time-stepping DG method (5) reduces to the implicit Euler scheme

$$\frac{U^n - U^{n-1}}{\Delta t} + AU^n = 0, \quad (8)$$

for which the following error bound holds [18, Theorems 7.1 and 7.2]:

$$\|U^n - u(t_n)\| \leq C t_n^{r-1} \Delta t \|A^r u_0\| \quad \text{for } n = 1, 2, 3, \dots \text{ and } 0 \leq r \leq 1. \quad (9)$$

This result is just the limiting case as $\nu \rightarrow 1$ of our error estimate (3) for the fractional diffusion equation.

For any real $r \geq 0$, we can characterize $D(A^r)$ in terms of the generalized Fourier coefficients in an eigenfunction expansion,

$$v = \sum_{m=1}^{\infty} v_m \phi_m, \quad v_m = \langle v, \phi_m \rangle.$$

Indeed, $v \in \mathcal{H}$ belongs to $D(A^r)$ if and only if

$$\|A^r v\|^2 = \sum_{m=1}^{\infty} \lambda_m^{2r} v_m^2 < \infty, \quad (10)$$

in which case the series $A^r v = \sum_{m=1}^{\infty} \lambda_m^r v_m \phi_m$ converges in \mathcal{H} . Thus (recalling our assumption that $\lambda_m \rightarrow \infty$) the larger the value of r such that $v \in D(A^r)$, the faster the Fourier coefficients v_m decay as $m \rightarrow \infty$ and the “smoother” v is. When $\mathcal{H} = L_2(\Omega)$ the functions in $D(A^r)$ may have to satisfy compatibility conditions on $\partial\Omega$; see Thomée [18, Lemma 3.1] or [10, Section 3]. In particular, an infinitely differentiable function will be somewhat “non-smooth” if it fails to satisfy the boundary conditions of our problem.

We note that, for a given u_0 , the exact solution u is less smooth than is the case for the classical heat equation. To see why, consider the Fourier expansion

$$u(t) = \sum_{m=1}^{\infty} u_m(t) \phi_m, \quad u_m(t) = \langle u(t), \phi_m \rangle, \quad (11)$$

and put $u_{0m} = \langle u_0, \phi_m \rangle$. The Fourier coefficients $u_m(t)$ satisfy the initial-value problem

$$u'_m + \lambda_m \partial_t^{1-\nu} u_m = 0, \quad \text{for } t > 0, \text{ with } u_m(0) = u_{0m}, \quad (12)$$

so that, as is well known [10], $u_m(t) = E_\nu(-\lambda_m t^\nu) u_{0m}$ where E_ν denotes the Mittag-Leffler function. Since $E_\nu(-s) = O(s^{-1})$ decays slowly as $s \rightarrow \infty$ for $0 < \nu < 1$, in comparison to $E_1(-s) = e^{-s}$, the high frequency modes of the solution are not damped as rapidly as in the classical case $\nu = 1$.

Section 2 uses Laplace transform techniques to derive integral representations for the Fourier coefficients $U_m^n = \langle U^n, \phi_m \rangle$ and $u_m(t_n) = \langle u(t_n), \phi_m \rangle$. We show that $U_m^n - u_m(t_n) = \delta^n(\mu) u_{0m}$, where $\delta^n(\mu)$ is given by an explicit but complicated integral; thus, the error has a Fourier expansion of the form

$$U^n - u(t_n) = \sum_{m=1}^{\infty} \delta^n(\lambda_m \Delta t^\nu) u_{0m} \phi_m, \quad u_{0m} = \langle u_0, \phi_m \rangle. \quad (13)$$

Theorem 4 states a key estimate for $\delta^n(\mu)$, but to avoid a lengthy digression the proof is relegated to Section 4.

The main result (3) of the paper is established in Section 3, where we first prove in Theorem 5 that if $u_0 \in \mathcal{H}$ then the error is of order $t_n^{-1}\Delta t$, coinciding with the error estimate (9) for the classical heat equation when $r = 0$. Next we prove the special case $r = \min(2, 1/\nu)$ of (3) and then, in Theorem 7, deduce the general case by interpolation. The paper concludes with Section 5, which presents the results of some computational experiments for a model 1D problem, as well as numerical evidence that the constant C in (3) can be chosen independent of ν .

2. Integral representations

Our error analysis relies on the Laplace transform

$$\hat{u}(z) = \mathcal{L}\{u(t)\} = \int_0^\infty e^{-zt} u(t) dt.$$

A standard energy argument [11, 13] shows that $\|u(t)\| \leq \|u_0\|$ so $\hat{u}(z)$ exists and is analytic in the right half-plane $\Re z > 0$, and since $\mathcal{L}\{\partial_t^{1-\nu} u\} = z^{1-\nu} \hat{u}(z)$ and $\mathcal{L}\{\partial_t u\} = z\hat{u} - u_0$, it follows from (12) that $z\hat{u}_m + \lambda_m z^{1-\nu} \hat{u}_m = u_{0m}$, so

$$\hat{u}_m(z) = \frac{u_{0m}}{z + \lambda_m z^{1-\nu}}.$$

Thus, the Laplace inversion formula gives, for $n \geq 1$ and any $a > 0$,

$$u_m(t_n) = \frac{1}{2\pi i} \int_{a-i\infty}^{a+i\infty} e^{zt_n} \hat{u}_m(z) dz = \frac{u_{0m}}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{e^{zt_n}}{1 + \lambda_m z^{-\nu}} \frac{dz}{z},$$

which, following a substitution, we may write as

$$u_m(t_n) = \frac{u_{0m}}{2\pi i} \int_{a-i\infty}^{a+i\infty} \frac{e^{nz}}{1 + \mu z^{-\nu}} \frac{dz}{z}, \quad \text{where } \mu = \lambda_m \Delta t^\nu. \quad (14)$$

It follows using Jordan's lemma that

$$u_m(t_n) = \frac{u_{0m}}{2\pi i} \int_{-\infty}^{0^+} \frac{e^{nz}}{1 + \mu z^{-\nu}} \frac{dz}{z} \quad \text{for } n \geq 1, \quad (15)$$

where the notation $\int_{-\infty}^{0^+}$ indicates that the path of integration is a Hankel contour enclosing the negative real axis and oriented counterclockwise.

Now consider the recurrence relation (6) used to compute the numerical solution. The Fourier coefficients $U_m^n = \langle U^n, \phi_m \rangle$ satisfy

$$(1 + \beta_0 \Delta t^\nu \lambda_m) U_m^n = U_m^{n-1} - \lambda_m \Delta t^\nu \sum_{j=1}^{n-1} \beta_{n-j} U_m^j, \quad (16)$$

and to obtain an integral representation of U_m^n analogous to (15) we introduce the discrete-time Laplace transform

$$\tilde{U}(z) = \sum_{n=0}^{\infty} U^n e^{-nz}. \quad (17)$$

Again, a standard energy argument shows that $\|U^n\| \leq \|u_0\|$ so this series converges in the right half-plane $\Re z > 0$. Multiplying (16) by e^{-nz} , summing over n and using the fact that the sum in (16) is a discrete convolution, we find that

$$[1 - e^{-z} + \mu \tilde{\beta}(z)] \tilde{U}_m(z) = [1 + \mu \tilde{\beta}(z)] u_{0m},$$

again with $\mu = \lambda_m \Delta t^\nu$. So, letting $\psi(z) = \tilde{\beta}(z)/(1 - e^{-z})$,

$$\tilde{U}_m(z) = u_{0m} \frac{1 + \mu \tilde{\beta}(z)}{1 - e^{-z} + \mu \tilde{\beta}(z)} = u_{0m} \frac{(1 - e^{-z})^{-1} + \mu \psi(z)}{1 + \mu \psi(z)}. \quad (18)$$

For our subsequent analysis we now establish key properties of the function $\psi(z)$.

Following appropriate shifts of the summation index, one finds that

$$\tilde{\beta}(z) = \sum_{n=0}^{\infty} \beta_n e^{-nz} = (e^z - 1)(1 - e^{-z}) \frac{\text{Li}_{-\nu}(e^{-z})}{\Gamma(1 + \nu)}, \quad (19)$$

where the polylogarithm [9, 19] is defined by $\text{Li}_p(z) = \sum_{n=1}^{\infty} z^n/n^p$ for $|z| < 1$ and $p \in \mathbb{C}$; thus,

$$\psi(z) = (e^z - 1) \frac{\text{Li}_{-\nu}(e^{-z})}{\Gamma(1 + \nu)} = \frac{1}{\Gamma(1 + \nu)} \left(1 + \sum_{n=1}^{\infty} [(n+1)^\nu - n^\nu] e^{-nz} \right). \quad (20)$$

From the identity

$$\frac{1}{n^p} = \frac{\Gamma(1-p)}{2\pi i} \int_{-\infty}^{0^+} e^{nw} w^{p-1} dw,$$

we find, after interchanging the sum and integral, that

$$\text{Li}_p(e^{-z}) = \frac{\Gamma(1-p)}{2\pi i} \int_{-\infty}^{0^+} \frac{w^{p-1} dw}{e^{z-w} - 1} \quad (21)$$

for $\Re z$ sufficiently large. Thus, $\text{Li}_p(e^{-z})$ possesses an analytic continuation to the strip $-2\pi < \Im z < 2\pi$ with a cut along the negative real axis $(-\infty, 0]$. It follows that $\psi(z)$ is analytic for z in the same cut strip, and moreover

$$\overline{\psi(z)} = \psi(\bar{z}) \quad \text{and} \quad \psi(z + 2\pi i) = \psi(z). \quad (22)$$

Lemma 1. *If $|\Im z| \leq \pi$ and $z \notin (-\infty, 0]$, then*

$$\psi(z) = \frac{\sin \pi \nu}{\pi} \int_0^\infty \frac{s^{-\nu}}{1 - e^{-z-s}} \frac{1 - e^{-s}}{s} ds \quad (23)$$

and $1 + \mu \psi(z) \neq 0$ for $0 < \mu < \infty$.

Proof. Given $z \notin (-\infty, 0]$, we can choose a Hankel contour that does not enclose z , and the formulae (20) and (21) then imply that

$$\psi(z) = \frac{e^z - 1}{2\pi i} \int_{-\infty}^{0^+} \frac{w^{-\nu-1} dw}{e^{z-w} - 1}.$$

Since

$$\frac{e^z - 1}{e^{z-w} - 1} = 1 + \frac{e^w - 1}{1 - e^{w-z}} \quad \text{and} \quad \int_{-\infty}^{0^+} w^{-\nu-1} dw = 0,$$

we have

$$\psi(z) = \frac{1}{2\pi i} \int_{-\infty}^{0^+} \frac{w^{-\nu}}{1 - e^{w-z}} \frac{e^w - 1}{w} dw.$$

Define contours along either side of the cut,

$$\mathcal{C}_{\pm} = \{se^{\pm i\pi} : \text{for } 0 < s < \infty\}, \quad (24)$$

so that $\arg(w) = \pm\pi$ if $w \in \mathcal{C}_{\pm}$. Noting that the integrand is $O(w^{-\nu})$ as $w \rightarrow 0$, we may collapse the Hankel contour into $\mathcal{C}^+ - \mathcal{C}^-$ to obtain (23).

The second part of the lemma amounts to showing that $\psi(z) \notin (-\infty, 0]$. If $x \geq 0$ and $\alpha_n = e^{-xn}[(n+1)^{\nu} - n^{\nu}]$, then

$$\psi(x + iy) = \frac{1}{\Gamma(1 + \nu)} \left(1 + \sum_{n=1}^{\infty} \alpha_n \cos ny - i \sum_{n=1}^{\infty} \alpha_n \sin ny \right). \quad (25)$$

The sequence α_n is convex and tends to zero, so [21, pp. 183 and 228]

$$\Re\psi(x + iy) \geq \frac{1}{2\Gamma(1 + \nu)} \quad \text{and} \quad \Im\psi(x + iy) < 0 \quad \text{for } x \geq 0 \text{ and } 0 < y < \pi,$$

and using (22) we find that $\Im\psi(x \pm i\pi) = 0$ for $-\infty < x < \infty$. The polylogarithm satisfies [19, Equation (3.1)]

$$\Im \text{Li}_p(e^{-z}) = \mp \frac{\pi s^{p-1}}{\Gamma(p)} \quad \text{if } z = se^{\pm i\pi} \text{ for } 0 < s < \infty,$$

so, using the identity $\Gamma(1 + \nu)\Gamma(1 - \nu) = \pi\nu / \sin \pi\nu$,

$$\Im\psi(se^{\pm i\pi}) = \mp(1 - e^{-s})s^{-\nu-1} \sin \pi\nu, \quad (26)$$

and in particular $\Im\psi(x + i0) < 0$ but $\Im\psi(x - i0) > 0$ for $-\infty < x < 0$, whereas $\Im\psi(x) = 0$ for $0 < x < \infty$. Applying the strong maximum principle for harmonic functions, we conclude that $\Im\psi(x + iy) \neq 0$ if $0 < |y| < \pi$. We saw above that $\Re\psi(x + iy) > 0$ if $x \geq 0$, and by (23),

$$\psi(x \pm i\pi) = \frac{\sin \pi\nu}{\pi} \int_0^{\infty} \frac{s^{-\nu}}{1 + e^{-x-s}} \frac{1 - e^{-s}}{s} ds > 0$$

for all real x , which completes the proof. \square

Since

$$\frac{1}{2\pi i} \int_{a-i\pi}^{a+i\pi} e^{(n-j)z} dz = \delta_{nj} = \begin{cases} 1, & \text{if } n = j, \\ 0, & \text{if } n \neq j, \end{cases}$$

we see from the definition (17) of \tilde{U}_m , after interchanging the sum and integral, that for any $a > 0$,

$$U_m^n = \frac{1}{2\pi i} \int_{a-i\pi}^{a+i\pi} e^{nz} \tilde{U}_m(z) dz. \quad (27)$$

Moreover, since

$$\frac{(1 - e^{-z})^{-1} + \mu\psi(z)}{1 + \mu\psi(z)} = 1 + \frac{(1 - e^{-z})^{-1} - 1}{1 + \mu\psi(z)} = 1 - \frac{1/(1 - e^z)}{1 + \mu\psi(z)},$$

the formula (18) for $\tilde{U}_m(z)$ implies that

$$U_m^n = \frac{u_{0m}}{2\pi i} \int_{a-i\pi}^{a+i\pi} \frac{e^{nz}}{1 + \mu\psi(z)} \frac{dz}{e^z - 1} \quad \text{for } n \geq 1. \quad (28)$$

The next lemma describes the asymptotic behaviour of ψ , and shows in particular that the integrands of (14) and (28) are close for z near 0. In (29), ζ denotes the Riemann zeta function.

Lemma 2. *The function (20) satisfies*

$$\psi(z) = z^{-\nu} + \frac{1}{2}z^{1-\nu} + \frac{\zeta(-\nu)}{\Gamma(1+\nu)} z + O(z^{2-\nu}) \quad \text{as } z \rightarrow 0, \quad (29)$$

and

$$\psi(z) = \frac{\sin \pi\nu}{\pi\nu} (i\pi - z)^{-\nu} + O(z^{-\nu-1}) \quad \text{as } \Re(z) \rightarrow -\infty, \text{ with } 0 < \Im z < \pi. \quad (30)$$

Proof. Flajolet [4, Theorem 1] shows that

$$\text{Li}_p(e^{-z}) \sim \Gamma(1-p)z^{p-1} + \sum_{k=0}^{\infty} (-1)^k \zeta(p-k) \frac{z^k}{k!} \quad \text{as } z \rightarrow 0, \quad (31)$$

and (29) follows because $e^z - 1 = z + \frac{1}{2}z^2 + O(z^3)$ as $z \rightarrow 0$. The results of Ford [5, Equation (17), p. 226] imply that

$$\text{Li}_p(e^{-z}) = -\frac{(i\pi - z)^p}{\Gamma(1+p)} + O(z^{p-1}) \quad \text{as } \Re z \rightarrow -\infty, \quad (32)$$

(see also Wood [19, Equation (11.2)]) which, in combination with the identity $\Gamma(1+\nu)\Gamma(1-\nu) = \pi\nu/\sin \pi\nu$, implies (30). \square

The formula for U_m^n in the next theorem matches (15) for $u_m(t_n)$.

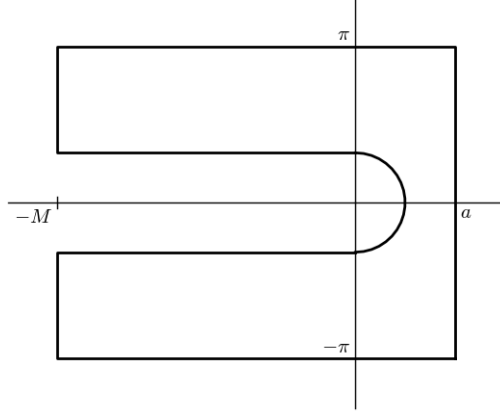


Figure 1: The integration contour $C(a, M)$.

Theorem 3. *The solution of (16) admits the integral representation*

$$U_m^n = \frac{u_{0m}}{2\pi i} \int_{-\infty}^{0^+} \frac{e^{nz}}{1 + \mu\psi(z)} \frac{dz}{e^z - 1} \quad \text{for } n \geq 1, \quad (33)$$

where the Hankel contour remains inside the strip $-\pi < \Im z < \pi$.

Proof. By Lemma 1, the integrand from (28) is analytic for z inside the contour $C(a, M)$ shown in Figure 1. The contributions along $\Im z = \pm\pi$ cancel in view of the second part of (22). Using (30), if $\Re z \rightarrow -\infty$ then

$$\frac{1/(e^z - 1)}{1 + \mu\psi(z)} \sim -\left(1 + \mu \frac{\sin \pi\nu}{\pi\nu} (i\pi - z)^{-\nu}\right)^{-1} \sim -1 + \mu \frac{\sin \pi\nu}{\pi\nu} (i\pi - z)^{-\nu},$$

so the contributions along $\Re z = -M$ are $O(e^{-nM})$ as $M \rightarrow \infty$, implying the desired formula for U_m^n . \square

Together, (15) and (33) imply that the error formula (13) holds, with

$$\delta^n(\mu) = \frac{1}{2\pi i} \int_{-\infty}^{0^+} e^{nz} \left(\frac{1}{1 + \mu\psi(z)} \frac{z}{e^z - 1} - \frac{1}{1 + \mu z^{-\nu}} \right) \frac{dz}{z} \quad (34)$$

for $0 < \mu < \infty$, and with $\delta^n(0) = 0$ because if $\lambda_m = 0$ then $u_m(t_n) = u_{0m} = U_m^n$ for all n . The following estimate for $\delta^n(\mu)$ is the key to proving our error estimates, but the lengthy proof is deferred until Section 4.

Theorem 4. *Let $0 < \nu < 1$. The sequence (34) satisfies*

$$|\delta^n(\mu)| \leq C n^{-1} \min((\mu n^\nu)^2, (\mu n^\nu)^{-1}) \quad \text{for } n = 1, 2, 3, \dots \text{ and } 0 < \mu < \infty.$$

Proof. Follows from Theorems 12 and 16. \square

We remark that in the limiting case $\nu \rightarrow 1$, when our method reduces to the classical implicit Euler scheme (8) for the heat equation (7), it is readily seen that the error representation (13) holds with $\delta^n(\mu) = (1 + \mu)^{-n} - e^{-n\mu}$, and that $0 \leq \delta^n(\mu) \leq Cn^{-1} \min((\mu n)^2, (\mu n)^{-1})$, consistent with Theorem 4.

3. Error estimates

We begin this section with the basic error bound that applies even when no smoothness is assumed for the initial data.

Theorem 5. *For any $u_0 \in \mathcal{H}$, the solutions of (1) and (5) satisfy*

$$\|U^n - u(t_n)\| \leq Ct_n^{-1} \Delta t \|u_0\| \quad \text{for } n = 1, 2, 3, \dots$$

Proof. Theorem 4 implies that $|\delta^n(\mu)| \leq Cn^{-1}$ uniformly for $0 < \mu < \infty$, and since the ϕ_m are orthonormal, we see from (13) that

$$\|U^n - u(t_n)\|^2 = \sum_{m=1}^{\infty} [\delta^n(\lambda_m \Delta t^\nu) u_{0m}]^2 \leq (Cn^{-1})^2 \sum_{m=1}^{\infty} u_{0m}^2 = (Cn^{-1} \|u_0\|)^2. \quad (35)$$

The estimate follows after recalling that $t_n = n\Delta t$ so $n^{-1} = t_n^{-1} \Delta t$. \square

For smoother initial data, the error bound exhibits a less severe deterioration as t_n approaches zero.

Lemma 6. *Consider the solutions of (1) and (5).*

1. *If $0 < \nu \leq 1/2$ and $A^2 u_0 \in \mathcal{H}$, then*

$$\|U^n - u(t_n)\| \leq Ct_n^{2\nu-1} \Delta t \|A^2 u_0\| \leq C \Delta t^{2\nu} \|A^2 u_0\|.$$

2. *If $1/2 \leq \nu < 1$ and $A^{1/\nu} u_0 \in \mathcal{H}$, then*

$$\|U^n - u(t_n)\| \leq C \Delta t \|A^{1/\nu} u_0\|.$$

Proof. In the first case, since $\lambda_m \Delta t^\nu n^\nu = \lambda_m t_n^\nu$,

$$\begin{aligned} |\delta^n(\lambda_m \Delta t^\nu)| &\leq Ct_n^{-1} \Delta t \min((\lambda_m t_n^\nu)^2, (\lambda_m t_n^\nu)^{-1}) \\ &= Ct_n^{2\nu-1} \Delta t \lambda_m^2 \min(1, (\lambda_m t_n^\nu)^{-3}) \leq Ct_n^{2\nu-1} \Delta t \lambda_m^2, \end{aligned}$$

so by (10) and (35),

$$\|U^n - u(t_n)\|^2 \leq \sum_{m=1}^{\infty} (Ct_n^{2\nu-1} \Delta t \lambda_m^2 u_{0m})^2 = (Ct_n^{2\nu-1} \Delta t \|A^2 u_0\|)^2,$$

with $t_n^{2\nu-1} \Delta t = n^{2\nu-1} \Delta t^{2\nu} \leq \Delta t^{2\nu}$. The second case follows in a similar fashion, because $n^{-1} = \Delta t \lambda_m^{1/\nu} (\lambda_m t_n^\nu)^{-1/\nu}$ implies that

$$|\delta^n(\lambda_m \Delta t^\nu)| \leq C \Delta t \lambda_m^{1/\nu} \min((\lambda_m t_n^\nu)^{2-1/\nu}, (\lambda_m t_n^\nu)^{-1-1/\nu}) \leq C \Delta t \lambda_m^{1/\nu}.$$

\square

We are now ready to prove our main result.

Theorem 7. *The solutions of (1) and (5) satisfy*

$$\|U^n - u(t_n)\| \leq C t_n^{r\nu-1} \Delta t \|A^r u_0\| \quad \text{for } 0 \leq r \leq \min(2, 1/\nu).$$

Proof. If $0 < \nu \leq 1/2$ and $0 < \theta < 1$, then by interpolation

$$\|U^n - u(t_n)\| \leq C (t_n^{-1} \Delta t)^{1-\theta} (t_n^{2\nu-1} \Delta t)^\theta \|A^{2\theta} u_0\| = C t_n^{2\nu\theta-1} \Delta t \|A^{2\theta} u_0\|,$$

and the estimate follows by putting $r = 2\theta$. Similarly, if $1/2 \leq \nu < 1$, then

$$\|U^n - u(t_n)\| \leq C (t_n^{-1} \Delta t)^{1-\theta} \Delta t^\theta \|A^{\theta/\nu} u_0\| = C t_n^{\theta-1} \Delta t \|A^{\theta/\nu} u_0\|,$$

and the estimate follows by putting $r = \theta/\nu$. \square

4. Technical proofs

It remains to prove Theorem 4. In this section only, C always denotes an absolute constant and we use subscripts in cases where the constant might depend on some parameters; for instance C_ν may depend on the fractional diffusion exponent ν .

Since the integrand of (34) is $O(z^{\nu-1})$ as $z \rightarrow 0$, we may collapse the Hankel contour onto $\mathcal{C}_+ - \mathcal{C}_-$, for \mathcal{C}_\pm given by (24). In this way, defining

$$\psi_\pm(s) = \psi(se^{\pm i\pi}) \quad \text{for } 0 < s < \infty,$$

we find that

$$\begin{aligned} \int_{\mathcal{C}_\pm} e^{nz} \left(\frac{1}{1 + \mu\psi(z)} \frac{z}{e^z - 1} - \frac{1}{1 + \mu z^{-\nu}} \right) \frac{dz}{z} \\ = \int_0^\infty e^{-ns} \left(\frac{1}{1 + \mu\psi_\pm(s)} \frac{s}{1 - e^{-s}} - \frac{1}{1 + \mu s^{-\nu} e^{\mp i\pi\nu}} \right) \frac{ds}{s}. \end{aligned}$$

By (22) and (26),

$$\psi_-(s) = \overline{\psi_+(s)} \quad \text{and} \quad \Im \psi_\pm(s) = \mp(1 - e^{-s})s^{-\nu-1} \sin \pi\nu, \quad (36)$$

so

$$\frac{1}{1 + \mu\psi_+(s)} - \frac{1}{1 + \mu\psi_-(s)} = \frac{2i\mu\Im\psi_-(s)}{|1 + \mu\psi_\pm(s)|^2} = \frac{2i\mu s^{-\nu} \sin \pi\nu}{|1 + \mu\psi_\pm(s)|^2} \frac{1 - e^{-s}}{s},$$

and similarly,

$$\frac{1}{1 + \mu s^{-\nu} e^{-i\pi\nu}} - \frac{1}{1 + \mu s^{-\nu} e^{i\pi\nu}} = \frac{2i\mu s^{-\nu} \sin \pi\nu}{|1 + \mu s^{-\nu} e^{\mp i\pi\nu}|^2}.$$

Thus, the representation (34) implies

$$\delta^n(\mu) = \frac{\sin \pi\nu}{\pi} \int_0^\infty e^{-ns} \mu s^{-\nu} \left(\frac{1}{|1 + \mu\psi_+(s)|^2} - \frac{1}{|1 + \mu s^{-\nu} e^{-i\pi\nu}|^2} \right) \frac{ds}{s}. \quad (37)$$

We will estimate this integral with the help of the following sequence of lemmas.

Lemma 8. *If $X \geq 0$ then $|1 + Xe^{\pm i\pi\nu}|^{-2} \leq (1 - \nu)^{-2}(1 + X^2)^{-1}$.*

Proof. Since $0 \leq 2X/(1 + X^2) \leq 1$,

$$\frac{|1 + Xe^{\pm i\pi\nu}|^2}{1 + X^2} = \frac{|e^{\mp i\pi\nu} + X|^2}{1 + X^2} = 1 + \frac{2X}{1 + X^2} \cos \pi\nu \geq \min(1, 1 + \cos \pi\nu),$$

and the result follows because $1 + \cos \pi\nu = 2 \cos^2(\pi\nu/2) \geq 2(1 - \nu)^2$. \square

Lemma 9. *If $\mu \geq 0$ and $s > 0$, then $|1 + \mu\psi_{\pm}(s)|^{-2} \leq C_{\nu}(1 + \mu^2 s^{-2\nu})^{-1}$.*

Proof. Lemma 2 implies that

$$\psi_{\pm}(s) = e^{\mp i\pi\nu}(s^{-\nu} - \frac{1}{2}s^{1-\nu}) - \frac{\zeta(-\nu)}{\Gamma(1+\nu)}s + O(s^{2-\nu}) \quad \text{as } s \rightarrow 0 \quad (38)$$

and

$$\psi_{\pm}(s) = \frac{\sin \pi\nu}{\pi\nu} s^{-\nu} + O(s^{-\nu-1}) \quad \text{as } s \rightarrow \infty. \quad (39)$$

Thus, if we define $\phi(s) = s^{\nu}\psi_{+}(s)$ for $0 < s < \infty$, with

$$\phi(0) = e^{-i\pi\nu} \quad \text{and} \quad \phi(\infty) = \frac{\sin \pi\nu}{\pi\nu}, \quad (40)$$

then ϕ is continuous on the one-point compactification $[0, \infty]$ of the closed half-line $[0, \infty)$. Put $X = \mu s^{-\nu}$ and define

$$f(s, X) = \frac{|1 + \mu\psi_{+}(s)|^2}{1 + X^2} = \frac{|1 + X\phi(s)|^2}{1 + X^2}$$

for $0 \leq s \leq \infty$ and $0 \leq X < \infty$, with $f(s, \infty) = |\phi(s)|^2$, so that f is continuous on the compact topological space $[0, \infty] \times [0, \infty]$. It therefore suffices to prove that f is strictly positive everywhere. By (36),

$$\Im \phi(s) = -\frac{1 - e^{-s}}{s} \sin \pi\nu < 0 \quad \text{for } 0 < s < \infty, \quad (41)$$

and $\Im \phi(0) = -\sin \pi\nu < 0$ by (40), so $|1 + X\phi(s)|^2 \geq [X\Im \phi(s)]^2 > 0$ for $0 \leq s < \infty$ and $0 < X < \infty$. Moreover, $|1 + X\phi(\infty)|^2 \geq 1$ because $\phi(\infty)$ is real and positive, and $f(s, 0) = 1$ for $0 \leq s \leq \infty$. Finally, (40) and (41) imply that $f(s, \infty) = |\phi(s)|^2 > 0$ for $0 \leq s \leq \infty$. \square

Lemma 10. *For $\mu \geq 0$ and $s > 0$,*

$$\begin{aligned} & |1 + \mu s^{-\nu} e^{\mp i\pi\nu}|^2 - |1 + \mu\psi_{\pm}(s)|^2 \\ &= \mu B_{+}(s)(1 + \mu s^{-\nu} e^{i\pi\nu}) + \mu B_{-}(s)(1 + \mu\psi_{+}(s)) = \mu B_1(s) + \mu^2 B_2(s), \end{aligned}$$

where $B_{\pm}(s) = s^{-\nu} e^{\mp i\pi\nu} - \psi_{\pm}(s)$ and

$$\begin{aligned} B_1(s) &= B_{+}(s) + B_{-}(s) = 2(s^{-\nu} \cos \pi\nu - \Re \psi_{\pm}(s)), \\ B_2(s) &= B_{+}(s)s^{-\nu} e^{i\pi\nu} + B_{-}(s)\psi_{+}(s) = s^{-2\nu} - \psi_{+}(s)\psi_{-}(s). \end{aligned}$$

Proof. Put $a = \mu s^{-\nu} e^{\mp i\pi\nu}$ and $b = \mu\psi_{\pm}$ in the identities

$$\begin{aligned} |1+a|^2 - |1+b|^2 &= (a-b)(1+\bar{a}) + (\bar{a}-\bar{b})(1+b) \\ &= (a-b) + (\bar{a}-\bar{b}) + (a\bar{a}-b\bar{b}). \end{aligned}$$

□

Notice that B_1 and B_2 are real, whereas $B_-(s) = \overline{B_+(s)}$.

Lemma 11. As $s \rightarrow 0$,

$$B_{\pm}(s) = O(s^{1-\nu}), \quad B_1(s) = s^{1-\nu} \cos \pi\nu + O(s), \quad B_2(s) = s^{1-2\nu} + O(s^{1-\nu}),$$

and as $s \rightarrow \infty$,

$$B_{\pm}(s) = O(s^{-\nu}), \quad B_1(s) = O(s^{-\nu}), \quad B_2(s) = O(s^{-2\nu}).$$

Proof. Follows using (38) and (39). □

We are now ready to prove the easier half of Theorem 4.

Theorem 12. For $0 < \mu < \infty$ and $n = 1, 2, 3, \dots$, the sequence (34) satisfies

$$|\delta^n(\mu)| \leq C_{\nu} n^{-1} \rho^{-1} \quad \text{if } \rho = \mu n^{\nu}.$$

Proof. From (37) and Lemma 10, we see that $\delta^n(\mu)$ equals

$$\frac{\sin \pi\nu}{\pi} \int_0^{\infty} e^{-ns} \mu s^{-\nu} \frac{\mu B_+(s)(1 + \mu s^{-\nu} e^{i\pi\nu}) + \mu B_-(s)(1 + \mu\psi_+(s))}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^2 |1 + \mu\psi_+(s)|^2} \frac{ds}{s},$$

and thus, by Lemmas 8 and 9,

$$|\delta^n(\mu)| \leq C_{\nu} \int_0^{\infty} e^{-ns} \mu s^{-\nu} \frac{\mu |B_{\pm}(s)|}{(1 + \mu^2 s^{-2\nu})^{3/2}} \frac{ds}{s}.$$

Lemma 11 implies that $|B_{\pm}(s)| \leq C_{\nu} \min(s^{1-\nu}, s^{-\nu}) = C_{\nu} s^{-\nu} \min(s, 1)$, so

$$|\delta^n(\mu)| \leq C_{\nu} \int_0^{\infty} g_n(s, \mu) ds \quad \text{where} \quad g_n(s, \mu) = e^{-ns} \mu^2 \frac{s^{-2\nu-1} \min(s, 1)}{(1 + \mu^2 s^{-2\nu})^{3/2}}.$$

The estimate for $\delta^n(\mu)$ follows because

$$\int_0^1 g_n(s, \mu) ds \leq \int_0^1 e^{-ns} \frac{s^{\nu}}{\mu} ds = \frac{n^{-1-\nu}}{\mu} \int_0^n e^{-s} s^{\nu} ds \leq \frac{\Gamma(1+\nu)}{n\rho}$$

and

$$\int_1^{\infty} g_n(s, \mu) ds \leq \int_1^{\infty} e^{-ns} \frac{s^{\nu-1}}{\mu} ds \leq \int_1^{\infty} \frac{e^{-ns}}{\mu} ds = \frac{n^{\nu}}{\rho} \frac{e^{-n}}{n} \leq \frac{C}{n\rho}.$$

□

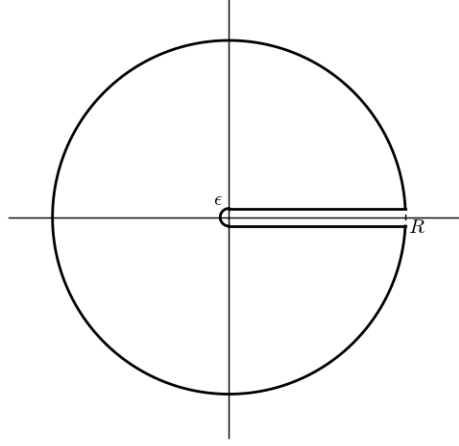


Figure 2: The contour $\mathcal{C}(\epsilon, R)$ used in the proof of Lemma 15.

Establishing the behaviour of $\delta^n(\mu)$ when $\rho = \mu n^\nu$ is small turns out to be more delicate, and relies on three additional lemmas.

Lemma 13. *If $0 \leq \nu \leq 1/2$ then $x^\nu \int_x^1 s^{-3\nu} ds \leq 3$ for $0 < x \leq 1$.*

Proof. Let $f(x) = x^\nu \int_x^1 s^{-3\nu} ds$. If $0 < \nu < 1/3$ then

$$f'(x) > 0 \text{ for } 0 < x < x^* \quad \text{and} \quad f'(x) < 0 \text{ for } x^* < x < 1, \quad (42)$$

where $x^* = [\nu/(1-2\nu)]^{1/(1-3\nu)} < 1$. Since $f'(x) = \nu x^{-1} f(x) - x^{-2\nu}$,

$$f(x) \leq f(x^*) = \frac{(x^*)^{1-2\nu}}{\nu} = \frac{(x^*)^\nu}{1-2\nu} \leq 3.$$

If $\nu = 1/3$, then $f(x) = x^{1/3} \log x^{-1}$ and (42) holds with $x^* = e^{-3}$, implying that $f(x) \leq f(x^*) = 3e^{-1} \leq 3$. If $1/3 < \nu < 1/2$, then (42) holds with $x^* = [(1-2\nu)/\nu]^{1/(3\nu-1)} < 1$ and again $f(x) \leq f(x^*) = (x^*)^{1-2\nu}/\nu \leq 3$. Finally, if $\nu = 0$ then $f(x) = 1 - x \leq 1$, and if $\nu = 1/2$ then $f(x) = 2(1 - x^{1/2}) \leq 2$. \square

Lemma 14. *If $1/2 \leq \nu \leq 1$ then $x^{\nu-1} \int_1^x s^{1-3\nu} ds \leq 3$ for $1 \leq x < \infty$.*

Proof. Make the substitutions $x' = x^{-1}$, $s' = s^{-1}$, $\nu' = 1 - \nu$ in Lemma 13. \square

Lemma 15. *If $1/2 < \nu < 1$ then*

$$\int_0^\infty \frac{s^{-2\nu} \cos \pi\nu + s^{-3\nu}}{|1 + s^{-\nu} e^{i\pi\nu}|^4} ds = \int_0^\infty \frac{s^\nu + s^{2\nu} \cos \pi\nu}{|s^\nu + e^{i\pi\nu}|^4} ds = 0.$$

Proof. Let $p = -\cos \pi\nu$ so that $0 < p < 1$. Making the substitution $x = s^\nu$, we see that the integral equals $\nu^{-1}I$, where

$$I = \int_0^\infty f(x) dx \quad \text{and} \quad f(x) = \frac{1 - px}{(x^2 - 2px + 1)^2} x^{1/\nu}.$$

We consider the analytic continuation of f to the cut plane $\mathbb{C} \setminus [0, \infty)$, and note that $z^2 - 2pz + 1 = (z - \alpha_+)(z - \alpha_-)$ where $\alpha_\pm = p \pm iq = e^{i\pi(1 \mp \nu)}$ and $q = \sqrt{1 - p^2} = \sin \pi\nu$. Thus, f has double poles at $z = \alpha_+$ and at α_- . Moreover, since $1 < 1/\nu < 2$ we see that $f(z) = o(|z|^{-1})$ as $|z| \rightarrow \infty$, and that $f(z) = O(|z|)$ as $|z| \rightarrow 0$. After integrating around the contour $\mathcal{C}(\epsilon, R)$ shown in Figure 2 and sending $\epsilon \rightarrow 0^+$ and $R \rightarrow \infty$, we conclude that

$$\frac{1 - e^{i2\pi/\nu}}{2\pi i} I = \operatorname{res}_{z=\alpha_+} f(z) + \operatorname{res}_{z=\alpha_-} f(z).$$

Since $(z - \alpha_\pm)^2 f(z) = (1 - pz)z^{1/\nu}/(z - \alpha_\mp)^2$ and $\alpha_+^{1/\nu} = -e^{i\pi/\nu} = \alpha_-^{1/\nu}$,

$$\operatorname{res}_{z=\alpha_\pm} f(z) = \lim_{z \rightarrow \alpha_\pm} \frac{d}{dz} (z - \alpha_\pm)^2 f(z) = \frac{d}{dz} \frac{(1 - pz)z^{1/\nu}}{(z - \alpha_\mp)^2} \Big|_{z=\alpha_\pm} = \mp i \frac{1 - \nu}{\nu} \frac{e^{i\pi/\nu}}{4q},$$

showing that the residues cancel, and therefore $I = 0$ because $e^{i2\pi/\nu} \neq 1$. \square

Our final result for this section completes the proof of Theorem 4, and hence of the error estimates of Section 3.

Theorem 16. *For $0 < \mu < \infty$ and $n = 1, 2, 3, \dots$, the sequence (34) satisfies*

$$|\delta^n(\mu)| \leq C_\nu n^{-1} \rho^2 \quad \text{if } \rho = \mu n^\nu \leq 1.$$

Proof. By Lemma 11,

$$\mu B_1(s) + \mu^2 B_2(s) = s(\mu s^{-\nu} \cos \pi\nu + (\mu s^{-\nu})^2 + O(\mu + \mu^2 s^{-\nu})) \quad \text{as } s \rightarrow 0^+,$$

and $\mu B_1(s) + \mu^2 B_2(s) = O(\mu s^{-\nu} + \mu^2 s^{-2\nu})$ as $s \rightarrow \infty$, so (37) implies that

$$\begin{aligned} |\delta^n(\mu)| &= \left| \frac{\sin \pi\nu}{\pi} \int_0^\infty e^{-ns} \mu s^{-\nu} \frac{\mu B_1(s) + \mu^2 B_2(s)}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^2 |1 + \mu \psi_+(s)|^2} \frac{ds}{s} \right| \\ &\leq \frac{\sin \pi\nu}{\pi} (|I_1| + C_\nu I_2 + C_\nu I_3), \end{aligned}$$

where, using Lemmas 8 and 9,

$$\begin{aligned} I_1 &= \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} \cos \pi\nu + (\mu s^{-\nu})^2}{|1 + \mu s^{-\nu} e^{i\pi\nu}|^2 |1 + \mu \psi_+(s)|^2} ds, \\ I_2 &= \int_0^1 e^{-ns} \mu s^{-\nu} \frac{\mu + \mu^2 s^{-\nu}}{(1 + \mu^2 s^{-2\nu})^2} ds, \quad I_3 = \int_1^\infty e^{-ns} \mu s^{-\nu} \frac{\mu s^{-\nu} + \mu^2 s^{-2\nu}}{(1 + \mu^2 s^{-2\nu})^2} \frac{ds}{s}. \end{aligned}$$

Put $f(x) = (x + x^2)/(1 + x^2)^2$ so that

$$I_2 = \mu \int_0^1 e^{-ns} f(\mu s^{-\nu}) ds = n^{-1-\nu} \rho \int_0^n e^{-s} f(\rho s^{-\nu}) ds.$$

Since $f(x) \leq \min(2x, x^{-2})$ we have $f(\rho s^{-\nu}) \leq C \min(\rho^{-2} s^{2\nu}, \rho s^{-\nu})$ and thus

$$\begin{aligned} n^{1+\nu} \rho^{-1} I_2 &\leq C \rho^{-2} \int_0^{\rho^{1/\nu}} e^{-s} s^{2\nu} ds + C \rho \int_{\rho^{1/\nu}}^n e^{-s} s^{-\nu} ds \\ &\leq C \int_0^{\rho^{1/\nu}} e^{-s} ds + C \rho \int_{\rho^{1/\nu}}^1 s^{-\nu} ds + C \rho \int_1^\infty e^{-s} ds \\ &\leq C \rho^{1/\nu} + C(1-\nu)^{-1} \rho + C \rho \leq C(1-\nu)^{-1} \rho + C \rho^{1/\nu} \leq C_\nu \rho, \end{aligned}$$

implying $I_2 \leq C_\nu n^{-1-\nu} \rho^2 \leq C_\nu n^{-1} \rho^2$. Noting that $\mu = \rho n^{-\nu} \leq 1$, we have

$$I_3 \leq \int_1^\infty e^{-ns} \mu^2 s^{-2\nu-1} ds \leq \mu^2 \int_1^\infty e^{-ns} ds = \mu^2 \frac{e^{-n}}{n} \leq n^{-1} \mu^2 = n^{-1-2\nu} \rho^2,$$

and therefore $I_3 \leq n^{-1} \rho^2$.

It remains to estimate I_1 . First consider the case $0 < \nu < 1/2$, in which $\cos \pi \nu > 0$. Put $g(x) = (x^2 \cos \pi \nu + x^3)/(1 + x^2)^2$, so that

$$I_1 \leq C_\nu \int_0^1 e^{-ns} g(\mu s^{-\nu}) ds = C_\nu n^{-1} \int_0^n e^{-s} g(\rho s^{-\nu}) ds.$$

Since $g(x) \leq \min(2x^2, x^{-2} \cos \pi \nu + x^{-1})$ we have

$$g(\rho s^{-\nu}) \leq C \min(\rho^{-1} s^\nu, \rho^2 s^{-2\nu} \cos \pi \nu + \rho^3 s^{-3\nu})$$

and hence $\int_0^n e^{-s} g(\rho s^{-\nu}) ds$ is bounded by

$$\begin{aligned} &C \rho^{-1} \int_0^{\rho^{1/\nu}} s^\nu ds + C \rho^2 \cos \pi \nu \int_{\rho^{1/\nu}}^n e^{-s} s^{-2\nu} ds + C \rho^3 \int_{\rho^{1/\nu}}^n e^{-s} s^{-3\nu} ds \\ &\leq C \rho^{1/\nu} + C \rho^2 \int_{\rho^{1/\nu}}^1 (1-2\nu) s^{-2\nu} ds + C \rho^3 \int_{\rho^{1/\nu}}^1 s^{-3\nu} ds + C \rho^2 \int_1^\infty e^{-s} ds. \end{aligned}$$

Applying Lemma 13 with $x = \rho^{1/\nu}$ and noting that $1/\nu > 2$, it follows that $\int_0^n e^{-s} g(\rho s^{-\nu}) ds \leq C(\rho^{1/\nu} + \rho^2)$ and hence $I_1 \leq C_\nu n^{-1} \rho^2$.

If $\nu = 1/2$, then $\cos \pi \nu = 0$ and the argument above again shows that $I_1 \leq C_\nu n^{-1} \rho^2$. Thus, assume now that $1/2 < \nu < 1$ and note $\cos \pi \nu < 0$. Since

$$\begin{aligned} \frac{e^{-ns}}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 |1 + \mu \psi_+(s)|^2} &= \frac{1}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^4} \\ &\quad - \frac{1 - e^{-ns}}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 |1 + \mu \psi_+(s)|^2} + \frac{|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 - |1 + \mu \psi_+(s)|^2}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^4 |1 + \mu \psi_+(s)|^2} \end{aligned}$$

and, by Lemma 15,

$$\begin{aligned} \int_0^1 \frac{(\mu s^{-\nu})^2 \cos \pi \nu + (\mu s^{-\nu})^3}{|1 + \mu s^{-\nu} e^{i\pi \nu}|^4} ds &= \mu^{1/\nu} \int_0^{\mu^{-1/\nu}} \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{|1 + s^{-\nu} e^{i\pi \nu}|^4} ds \\ &= -\mu^{1/\nu} \int_{\mu^{-1/\nu}}^\infty \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{|1 + s^{-\nu} e^{i\pi \nu}|^4} ds, \end{aligned}$$

we have

$$|I_1| \leq C_\nu (J_1 + J_2 + J_3), \quad (43)$$

where

$$\begin{aligned} J_1 &= \mu^{1/\nu} \int_{\mu^{-1/\nu}}^\infty \frac{s^{-2\nu} \cos \pi \nu + s^{-3\nu}}{(1 + \mu^2 s^{-2\nu})^2} ds, \\ J_2 &= \int_0^1 (1 - e^{-ns}) \frac{(\mu s^{-\nu})^2 |\cos \pi \nu| + (\mu s^{-\nu})^3}{(1 + \mu^2 s^{-2\nu})^2} ds, \\ J_3 &= \int_0^1 (|1 + \mu s^{-\nu} e^{i\pi \nu}|^2 - |1 + \mu \psi_+(s)|^2) \frac{(\mu s^{-\nu})^2 |\cos \pi \nu| + (\mu s^{-\nu})^3}{(1 + \mu^2 s^{-2\nu})^3} ds. \end{aligned}$$

First, because $\mu^{1/\nu} = n^{-1} \rho^{1/\nu}$ and $|\cos \pi \nu| = \sin \pi(\nu - \frac{1}{2}) \leq \pi(\nu - \frac{1}{2})$,

$$\begin{aligned} J_1 &\leq C n^{-1} \rho^{1/\nu} \int_{n\rho^{-1/\nu}}^\infty ((2\nu - 1)s^{-2\nu} + s^{-3\nu}) ds \\ &\leq C n^{-1} \rho^{1/\nu} [(n\rho^{-1/\nu})^{1-2\nu} + (n\rho^{-1/\nu})^{1-3\nu}] \\ &= C n^{-2\nu} \rho^2 + C n^{-3\nu} \rho^3 \leq C n^{-1} \rho^2. \end{aligned}$$

Second, since $1 - e^{-x} \leq x$ and $\mu^{-1/\nu} = n\rho^{-1/\nu} \geq 1$, we see that $n\rho^{-1/\nu} J_2$ equals

$$\begin{aligned} \int_0^{n\rho^{-1/\nu}} (1 - e^{-\rho^{1/\nu} s}) \frac{s^{-2\nu} |\cos \pi \nu| + s^{-3\nu}}{(1 + s^{-2\nu})^2} ds &\leq C \int_0^1 \frac{(1 - e^{-\rho^{1/\nu} s}) s^{-3\nu}}{(1 + s^{-2\nu})^2} ds \\ &\quad + C \int_1^{n\rho^{-1/\nu}} (1 - e^{-\rho^{1/\nu} s}) (s^{-2\nu}(\nu - \frac{1}{2}) + s^{-3\nu}) ds \\ &\leq C \rho^{1/\nu} \int_0^1 s^{\nu+1} ds + C \int_{\rho^{1/\nu}}^n (1 - e^{-s}) (\rho^3 s^{-3\nu} + (\nu - \frac{1}{2}) \rho^2 s^{-2\nu}) ds. \end{aligned}$$

Since $\rho^3 s^{-3\nu} \leq \rho^2 s^{-2\nu}$ for $s \geq \rho^{1/\nu}$, the last integral is bounded by

$$\begin{aligned} \int_{\rho^{1/\nu}}^1 2\rho^2 s^{1-2\nu} ds + C \int_1^n (2\nu - 1) (\rho^3 s^{-3\nu} + \rho^2 s^{-2\nu}) ds \\ \leq C \int_{\rho^{1/\nu}}^1 \rho^2 s^{-1} ds + C \rho^3 + C \rho^2 \leq C \rho^{3-1/\nu} + C \rho^2 \log \rho^{-1/\nu}, \end{aligned}$$

and thus

$$J_2 \leq C n^{-1} \rho^{1/\nu} (\rho^{1/\nu} + C \rho^{3-1/\nu} + \nu^{-1} \rho^2 \log \rho^{-1}) \leq C_\nu n^{-1} \rho^2.$$

Third, by Lemmas 10 and 11,

$$\begin{aligned}
J_3 &\leq \int_0^1 (\mu s^{1-\nu} + \mu^2 s^{1-2\nu}) \frac{(\mu s^{-\nu})^2 + (\mu s^{-\nu})^3}{(1 + \mu s^{-\nu})^3} ds \\
&= \mu^{1+1/\nu} \int_0^{\mu^{-1/\nu}} \frac{s(s^{-\nu} + s^{-2\nu})(s^{-2\nu} + s^{-3\nu})}{(1 + s^{-2\nu})^3} ds \\
&\leq (\rho n^{-\nu})^{1+1/\nu} \left(\int_0^1 s^{1+\nu} ds + \int_1^{n\rho^{-1/\nu}} s^{1-3\nu} ds \right),
\end{aligned}$$

and applying Lemma 14 with $x = n\rho^{-1/\nu}$ gives $\int_1^{n\rho^{-1/\nu}} s^{1-3\nu} ds \leq 3(n\rho^{-1/\nu})^{1-\nu}$ so $J_3 \leq Cn^{-\nu-1}\rho^{1+1/\nu}(1+n^{1-\nu}\rho^{1-1/\nu}) \leq C(n^{-\nu-1}\rho^{1+1/\nu}+n^{-2\nu}\rho^2) \leq Cn^{-1}\rho^2$. Inserting the foregoing estimates for J_1 , J_2 and J_3 into (43) gives the desired estimate $|I_1| \leq Cn^{-1}\rho^2$, which completes the proof. \square

5. Numerical example

We consider a 1D example in which $u = u(x, t)$ satisfies (1) with $Au = -(\kappa u_x)_x$ for $x \in \Omega = (-1, 1)$, subject to homogeneous Dirichlet boundary conditions $u(\pm 1, t) = 0$ for $0 < t \leq 1$. We choose $\kappa = 4/\pi^2$ so the orthonormal eigenfunctions and corresponding eigenvalues of A are

$$\phi_m(x) = \sin \frac{m\pi}{2}(x+1) \quad \text{and} \quad \lambda_m = m^2 \quad \text{for } m = 1, 2, 3, \dots$$

For our initial data we choose simply the constant function $u_0(x) = \pi/4$, which has the Fourier sine coefficients

$$u_{0m} = \langle u_0, \phi_m \rangle = \begin{cases} m^{-1}, & m = 1, 3, 5, \dots, \\ 0, & m = 2, 4, 6, \dots \end{cases}$$

Although infinitely differentiable, the function u_0 is “non-smooth” because it fails to satisfy the boundary conditions, and as a result the solution $u(x, t)$ is discontinuous at $x = \pm 1$ when $t = 0$. In fact, if $r < 1/4$ then

$$\|A^r u_0\|^2 = \sum_{m=1}^{\infty} (\lambda_m^r u_{0m})^2 = \sum_{j=1}^{\infty} (2j-1)^{4r-1} \leq \frac{C}{1-4r},$$

but if $r \geq 1/4$ then $u_0 \notin D(A^r)$.

Using a closed form expression for $\hat{u}(x, z)$, we construct a reference solution by applying a spectrally accurate numerical method [12] for inversion of the Laplace transform. To compute the discrete-time solution U^n we discretize also in space using piecewise linear finite elements on a fixed nonuniform mesh with M subintervals. In view of the discontinuity in the solution when $t = 0$, we concentrate the spatial grid points near $x = \pm 1$, but always use a constant timestep $\Delta t = 1/N$.

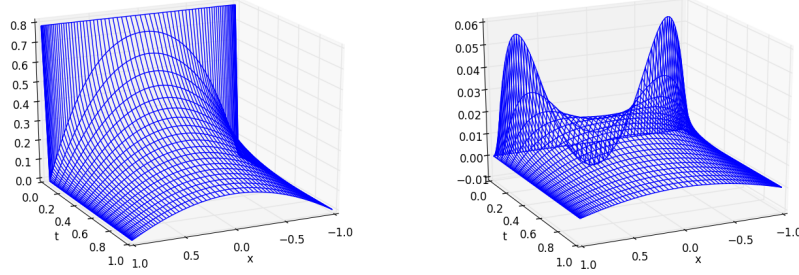


Figure 3: Reference solution (left) and error (right).

N	$\alpha = 0.6$		$\alpha = 0.7$		$\alpha = 13/16$	
80	2.14e-03		1.48e-03		1.16e-03	
160	1.24e-03	0.788	7.94e-04	0.894	5.91e-04	0.978
320	7.20e-04	0.787	4.29e-04	0.888	2.98e-04	0.988
640	4.17e-04	0.787	2.32e-04	0.887	1.50e-04	0.992
1280	2.42e-04	0.787	1.25e-04	0.887	7.53e-05	0.993

Table 1: Weighted errors and observed convergence rates from (44).

Figure 3 shows the reference solution and the error in the case $\nu = 0.75$ using $N = 20$ time steps and $M = 80$ spatial subintervals. As expected, the error is largest at the first time level t_1 and then decays as t increases. We put $r = \frac{1}{4} - \epsilon$ where $\epsilon^{-1} = \max(4, \log t_n^{-1})$, so that $t_n^{-\epsilon} \leq C$ and, by Theorem 7,

$$\|U^n - u(t_n)\| \leq C t_n^{\nu/4-1} \Delta t \sqrt{\max(1, \log t_n^{-1})} \quad \text{for } 0 < t_n \leq 1.$$

Thus, ignoring the logarithm and putting $\nu = 3/4$, we expect to observe errors of order $t_n^{-13/16} \Delta t$.

Figure 4 shows how the error varies with t_n for a sequence of solutions obtained by successively doubling N (and hence halving Δt), using a log scale. (The same spatial mesh with $M = 1000$ subintervals was used in all cases.) Table 1 provides an alternative view of this data, listing the weighted error and its associated convergence rate,

$$E_N = \max_{1 \leq t_n \leq 1/2} t_n^\alpha \|U^n - u(t_n)\| \quad \text{and} \quad \rho_N = \log_2(E_N/E_{N/2}), \quad (44)$$

so that if E_N decays like $N^{-\rho} = \Delta t^\rho$ then $\rho \approx \rho_N$. As expected, $\rho_N \approx 1$ when $\alpha = 13/16 = 0.8125$, but the rate deteriorates for smaller values of α .

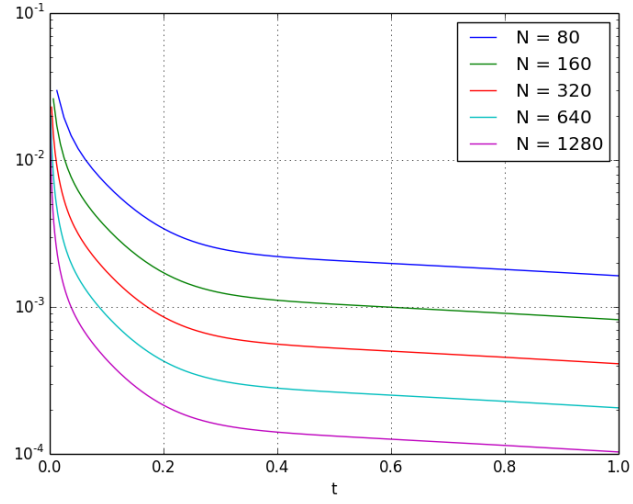


Figure 4: The error $\|U^n - u(t_n)\|$ as a function of t_n .

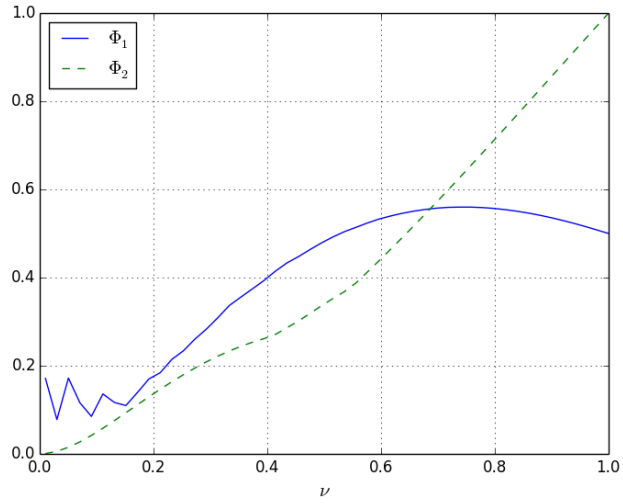


Figure 5: The functions Φ_1 and Φ_2 from (45).

Our analysis in Section 4 does not reveal how the constant in Theorem 4 depends on the fractional diffusion exponent ν , because the proof of Lemma 9 is not constructive. The factor $(1 - \nu)^{-2}$ in the estimate of Lemma 8 raises the question of whether the DG error becomes large if ν is very close to 1. We therefore investigated numerically the values of

$$\begin{aligned}\Phi_1(\nu) &= \sup_{0 < \mu < \infty} \max_{n^\nu \leq \mu^{-1}} n^{1-2\nu} \mu^{-2} \delta^n(\mu), \\ \Phi_2(\nu) &= \sup_{0 < \mu < \infty} \sup_{n^\nu \geq \mu^{-1}} n^{1+\nu} \mu \delta^n(\mu),\end{aligned}\tag{45}$$

since $C = \max(\Phi_1(\nu), \Phi_2(\nu))$ is the best possible constant in Theorem 4. Figure 5 shows approximations of the graphs of Φ_1 and Φ_2 , obtained by restricting μ to the discrete values 2^j for $-18 \leq j \leq 20$, and restricting n to the range $1 \leq n \leq 200$. We solved (12) and (16) with $u_{0m} = 1 = U_m^0$ and $\lambda_m = \mu/\Delta t^\nu$ to compute $\delta^n(\mu) = U_m^n - u_m(t_n)$. The evaluation of $\Phi_1(\nu)$ is problematic for ν near zero because our values for $u_m(t_n)$ are not sufficiently accurate, but it seems reasonable to conjecture that $C \leq 1$ for all ν .

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